Structural Studies of Organic Crystals of Pharmaceutical Relevance

Correlation of crystal structure analysis with recognised non-bonded structural motifs in the organic solid state

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ABSTRACT

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Pharmaceutical solids tend to exist in different physical forms termed as polymorphs. Issues about pharmaceutical systems are mainly concerned with the active ingredient's physico-chemical stability and bioavailability.

The main aim of this study is to investigate the non-bonded interactions in pharmaceutical solids that govern the physical pharmaceutics performance of such materials and through the use of structural techniques and correlation of these results with crystal structural database to establish the presence of physical motifs in selected systems. Structural motifs were identified by the use of single crystal and crystal packing analysis on diverse range of pharma-relevant materials including chalcones, cryptolepines, biguanides and xanthines. These selected systems were validated using functional group and molecular analysis and correlating them to the Cambridge Structural Database. Crystallization studies are done on these selected systems as well as exploiting those using synthetic analogues.

A total of 51 crystal structures were investigated including 16 new structure determinations. Addition synthesis of new xanthines to investigate novel intermolecular patterns was also undertaken. The understanding and exploitation of intermolecular interactions involving hydrogen bonds and coordination complexation during packing can be used in the design and synthesis of solid state molecular structures with desired physical and chemical properties.

TABLE OF CONTENTS

TABLE OF FIGURES

TABLE OF TABLES

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DEDICATION

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